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Phonon Transport in Semiconductor interface: An atomistic approach YANN CHALOPIN, MIT — Thermal dissipation and thermal insulation are among crucial issues encountered in high speed electronics devices and thermoelectrics systems. Both applications rely on controlling the transport properties of the heat carriers at semiconductor interfaces. From microscopic perspective, it is of fundamental interest to understand how the transport of phonons is impacted by an interface formed by two semiconductor layers. In a typical junction, the mechanism of reflection/transmission of vibrational energy causes strong modifications in the conductance regime. Thus, it is important to address the thermal transport at a contact junction in the framework of phonon wave propagation. Our approach is based on the fluctuation/dissipation theorem in order to calculate the thermal conductance of an interface. Using molecular dynamics simulations, we address the problems associated to using Si/Ge Si/SiGe junctions. We propose a methodology that enables the recovery of the transmission of the phonon modes by correlating the atomic motions of the phonon modes. Furthermore, we conclude that the phonon transmission function can be reconstructed such that it is integrated in the spectral expression of the conductance.

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